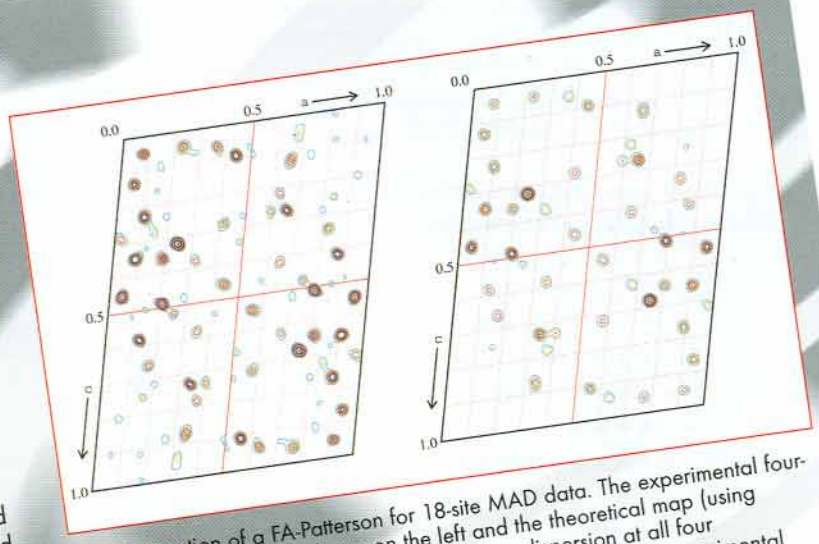
XPREP
RECIPROCAL SPACE EXPLORATION for MACROMOLECULES

The program XPREP, for years a mainstay of the Bruker SHELXTL system for small-molecule crystal structure determination, has been enhanced to make it equally useful for macromolecules.

XPREP can read single crystal diffraction data in a variety of different formats (SHELX .hkl files, SAINT .raw files, HKL2000 .sca files, XGEN .muf and .mui etc.) and can also generate ideal data (including anomalous contributions) from the atomic coordinates etc. These data may be transformed, scaled, merged and analyzed in a variety of different ways. XPREP is valid for all space groups.



Harker section of a FA-Patterson for 18-site MAD data. The experimental four-wavelength MAD map is shown on the left and the theoretical map (using XPREP to generate ideal data taking anomalous dispersion at all four wavelengths into account and deriving the FA-values as for the experimental data) is shown on the right.

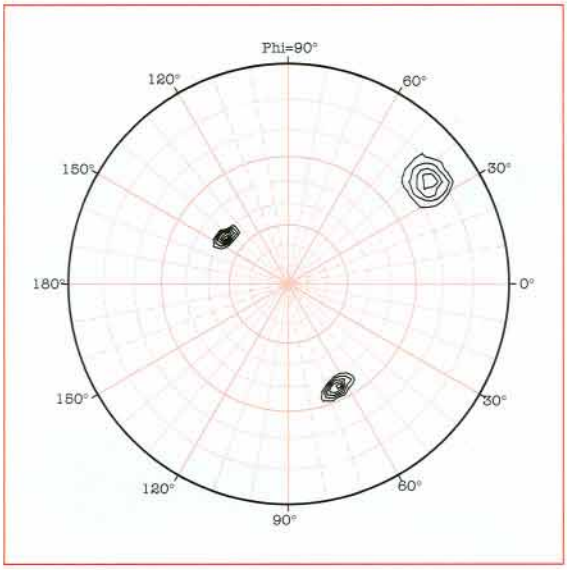
Key options include:

- Automatic space-group determination, if necessary transforming to a standard unit-cell in the process.
- All operations can handle reflections in any order and take equivalents into account, using the space group to distinguish between Friedel mates and true symmetry equivalents.
- Reciprocal space displays, with or without generation of symmetry equivalent reflections. This is useful for checking for data completeness and other artifacts.
- Processing of MAD, SIR, SAD and SIRAS data.

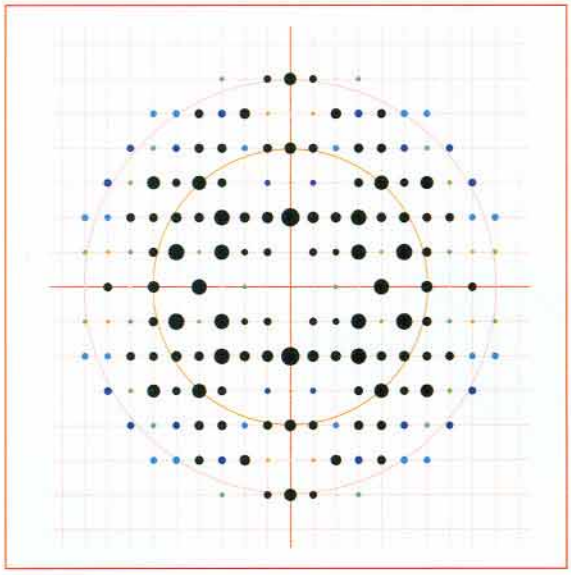
- Patterson Harker sections and peaklists. This is especially useful for checking heavy atom derivative data.
- Self-rotation functions to search for non-crystallographic symmetry. These can also be used to detect twinning.
- Detection of all types of merohedral twinning with estimates of the twin ratio.
- Optional renormalization of the intensity standard deviations, based on the agreement of equivalent reflections.
- Generation of free R flags either randomly or in thin shells and transfer of free R flags from one dataset to another. It does not matter which part of reciprocal space the reflections are taken from, and if equivalent reflections are present they are flagged consistently.
- Face-indexed and empirical corrections for absorption.
- Simulation of powder diffraction patterns using either the experimental single crystal data or data generated from the atomic coordinates.
- Preparation of input files for various programs including SHELX, CNS and X-PLOR.

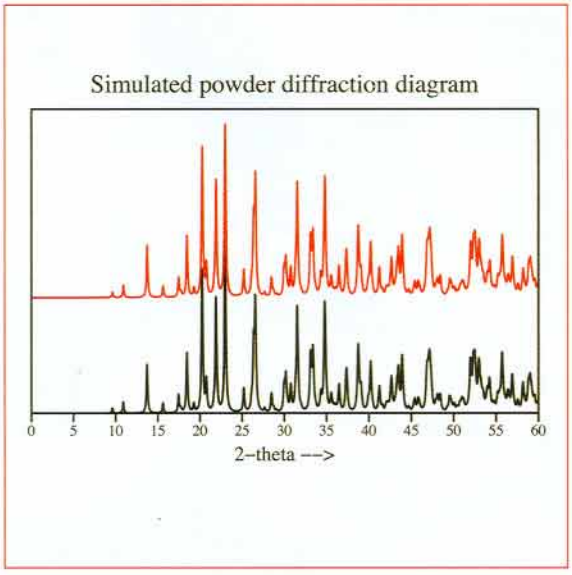
All graphical output may be stored as Postscript files as well as being displayed on the screen.

843-014300 for PC Windows
843-014500 for LINUX PC
843-014600 for SGI IRIX



Self-rotation function of a triclinic protein showing three two-fold axes 90 degrees from each other (local 222 non-crystallographic symmetry).





Reciprocal space display and simulated powder patters (above from the atomic coordinates, below from the experimental X-ray data) for the same small molecule.

BRUKER AXS INC.
5465 EAST CHERYL PARKWAY
MADISON, WI 53711
USA
TEL: 608-276-3000
FAX: 608-276-3006
E-mail: info@bruker-axs.com
http://www.bruker-axs.com

BRUKER NONIUS BV
OOSTSINGEL 209
2612 HL DELFT
THE NETHERLANDS
TEL: (+31) 15 215 24 00
FAX: (+31) 15 215 25 00
E-mail: info@bruker-nonius.com
http://www.bruker-nonius.com

BRUKER AXS GMBH
ÖSTLICHE RHEINBRÜCKENSTR. 49
D-76181 KARLSRUHE
GERMANY
TEL: (+49) 721-595-2888
FAX: (+49) 721-595-4587
E-mail: info@bruker-axs.de
http://www.bruker-axs.de